



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:08 PM UTC

PDB ID : 4MRO / pdb_00004mro
Title : Human GKRP bound to AMG-5980 and S6P
Authors : St Jean, D.J.; Ashton, K.S.; Bartberger, M.D.; Chen, J.; Chmait, S.; Cupples, R.; Galbreath, E.; Helmering, J.; Jordan, S.R.; Liu, L.; Kunz, K.; Michelsen, K.; Nishimura, N.; Pennington, L.D.; Poon, S.F.; Sivits, G.; Stec, M.M.; Tamayo, N.; Van, G.; Yang, K.; Norman, M.H.; Fotsch, C.; Lloyd, D.J.; Hale, C.
Deposited on : 2013-09-17
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

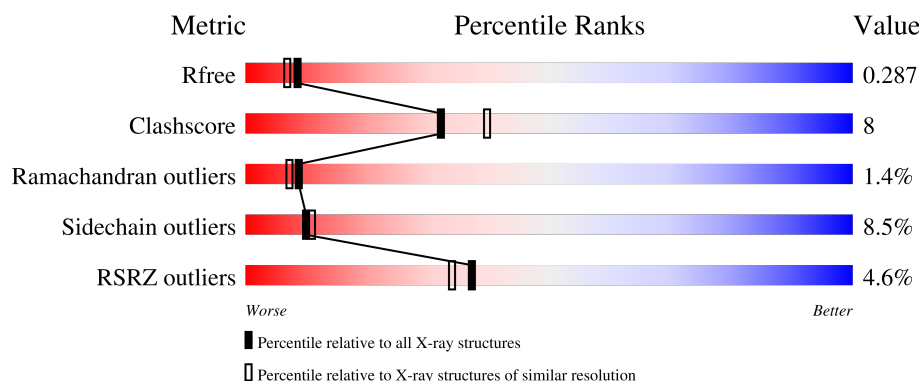
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	636	
1	B	636	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	B	712	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9286 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

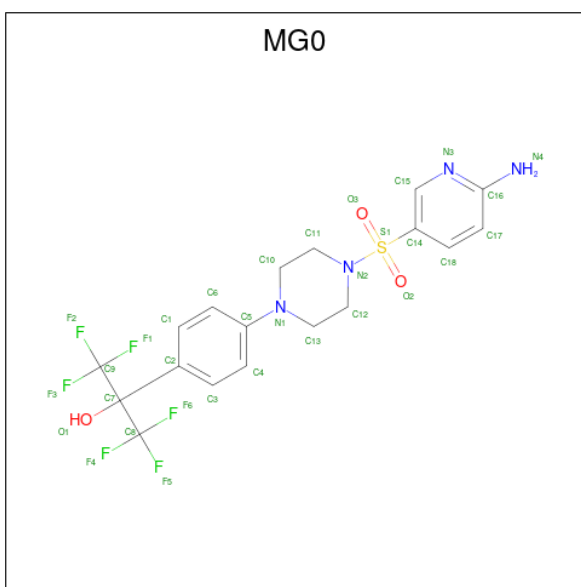
- Molecule 1 is a protein called Glucokinase regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4521	2882	774	841	24			
1	B	590	Total	C	N	O	S	0	0	0
			4554	2901	781	848	24			

There are 22 discrepancies between the modelled and reference sequences:

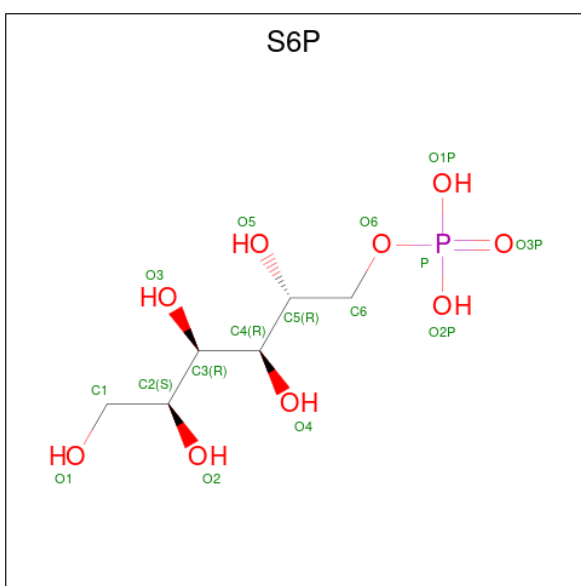
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression tag	UNP Q14397
A	-4	HIS	-	expression tag	UNP Q14397
A	-3	ASP	-	expression tag	UNP Q14397
A	-2	GLU	-	expression tag	UNP Q14397
A	-1	VAL	-	expression tag	UNP Q14397
A	0	ASP	-	expression tag	UNP Q14397
B	-10	MET	-	expression tag	UNP Q14397
B	-9	HIS	-	expression tag	UNP Q14397
B	-8	HIS	-	expression tag	UNP Q14397
B	-7	HIS	-	expression tag	UNP Q14397
B	-6	HIS	-	expression tag	UNP Q14397
B	-5	HIS	-	expression tag	UNP Q14397
B	-4	HIS	-	expression tag	UNP Q14397
B	-3	ASP	-	expression tag	UNP Q14397
B	-2	GLU	-	expression tag	UNP Q14397
B	-1	VAL	-	expression tag	UNP Q14397
B	0	ASP	-	expression tag	UNP Q14397

- Molecule 2 is 2-(4-{4-[(6-aminopyridin-3-yl)sulfonyl]piperazin-1-yl}phenyl)-1,1,1,3,3,3-hexafluoropropan-2-ol (CCD ID: MG0) (formula: C₁₈H₁₈F₆N₄O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			32	18	6	4	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			32	18	6	4	3	1		

- Molecule 3 is D-SORBITOL-6-PHOSPHATE (CCD ID: S6P) (formula: $C_6H_{15}O_9P$).

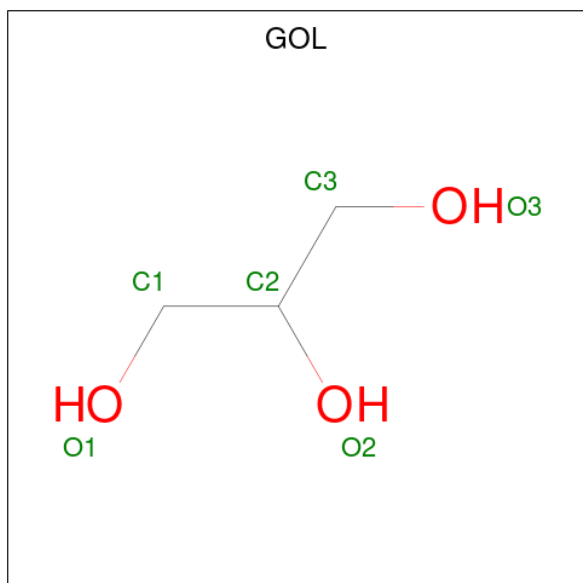


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

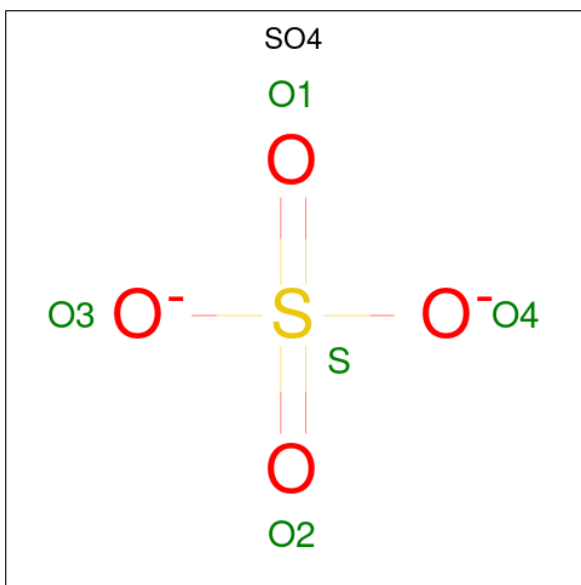
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	I	0	0
			11	11		
4	B	14	Total	I	0	0
			14	14		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

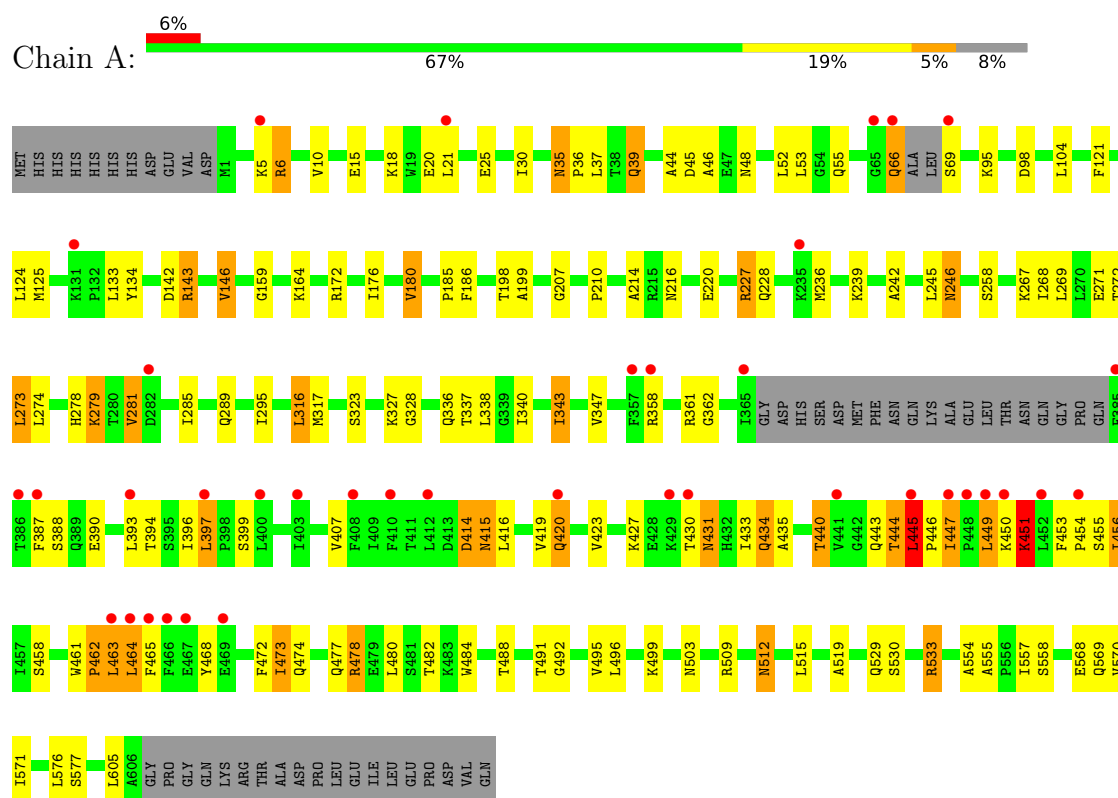
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	26	Total	O	0	0
			26	26		
7	B	43	Total	O	0	0
			43	43		

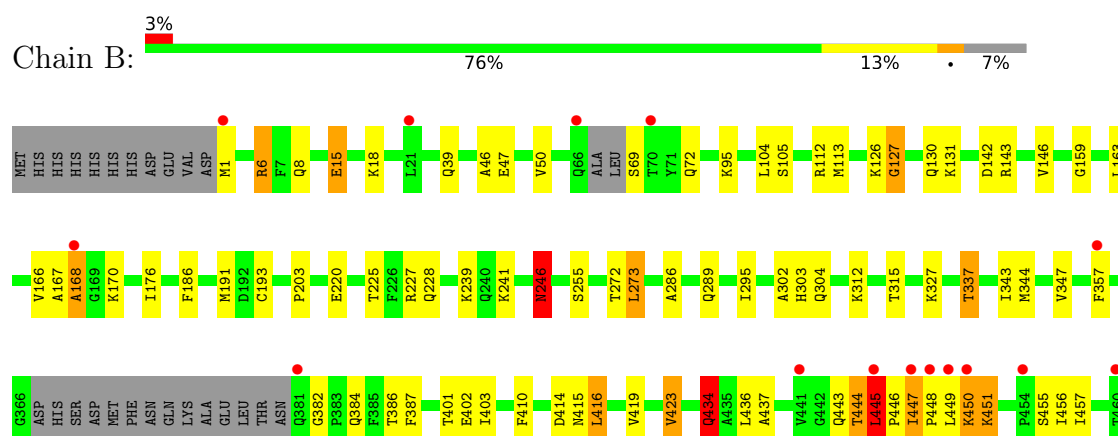
3 Residue-property plots

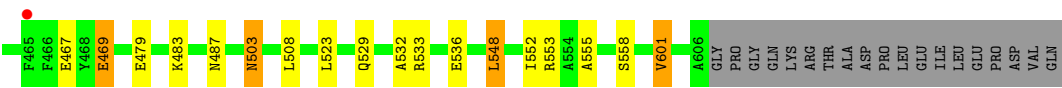
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glucokinase regulatory protein



• Molecule 1: Glucokinase regulatory protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	149.13Å 149.13Å 132.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.00 – 2.20 26.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.3 (26.00-2.20) 90.3 (26.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.230 , 0.288 0.236 , 0.287	Depositor DCC
R_{free} test set	3826 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG0, IOD, GOL, SO4, S6P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	3/4603 (0.1%)	1.15	9/6228 (0.1%)
1	B	1.12	5/4637 (0.1%)	1.15	15/6274 (0.2%)
All	All	1.12	8/9240 (0.1%)	1.15	24/12502 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	VAL	C-O	-5.88	1.18	1.24
1	B	436	LEU	CA-C	-5.84	1.46	1.53
1	A	216	ASN	C-O	-5.61	1.16	1.24
1	A	180	VAL	N-CA	-5.57	1.40	1.46
1	B	255	SER	CA-C	-5.39	1.45	1.52
1	B	203	PRO	C-O	-5.12	1.18	1.23
1	B	434	GLN	CD-NE2	-5.09	1.22	1.33
1	B	142	ASP	CA-C	-5.05	1.46	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	LYS	N-CA-C	-7.49	102.38	112.26
1	A	414	ASP	N-CA-C	7.34	122.65	112.45
1	B	434	GLN	N-CA-C	-7.08	98.31	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	GLN	N-CA-C	-6.99	100.11	110.46
1	B	444	THR	N-CA-C	6.45	120.77	112.12
1	A	20	GLU	N-CA-C	5.94	117.44	110.97
1	B	434	GLN	CB-CG-CD	5.82	122.49	112.60
1	A	443	GLN	N-CA-C	-5.76	102.38	110.50
1	A	279	LYS	CB-CA-C	5.73	119.97	110.81
1	B	163	LEU	N-CA-C	-5.68	105.00	111.14
1	A	343	ILE	N-CA-C	-5.54	105.32	110.53
1	B	382	GLY	CA-C-N	-5.53	114.01	119.92
1	B	382	GLY	C-N-CA	-5.53	114.01	119.92
1	B	601	VAL	CB-CA-C	-5.52	104.90	111.97
1	B	227	ARG	CB-CG-CD	-5.44	98.78	111.30
1	A	435	ALA	N-CA-C	5.28	116.87	108.79
1	A	440	THR	CB-CA-C	5.28	118.45	109.53
1	B	170	LYS	N-CA-C	-5.19	103.55	110.55
1	B	246	ASN	N-CA-C	5.17	117.54	108.75
1	A	449	LEU	CA-CB-CG	5.09	134.12	116.30
1	B	552	ILE	N-CA-C	-5.09	105.58	110.72
1	B	423	VAL	CB-CA-C	-5.07	105.22	112.22
1	B	105	SER	N-CA-C	5.04	117.66	109.24
1	B	357	PHE	N-CA-C	5.03	118.19	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4618	94	0
1	B	4554	0	4647	57	0
2	A	32	0	18	0	0
2	B	32	0	18	0	0
3	A	16	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	13	0	0
4	A	11	0	0	1	0
4	B	14	0	0	5	0
5	A	6	0	8	0	0
6	B	15	0	0	0	0
7	A	26	0	0	0	0
7	B	43	0	0	0	0
All	All	9286	0	9335	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HG22	1:A:449:LEU:C	2.01	0.84
1:B:419:VAL:O	1:B:423:VAL:HG23	1.79	0.83
1:B:445:LEU:HD13	1:B:450:LYS:HB3	1.61	0.82
1:A:447:ILE:HG22	1:A:450:LYS:N	1.99	0.78
1:B:225:THR:H	1:B:228:GLN:HE21	1.35	0.73
1:A:15:GLU:H	1:A:18:LYS:HE2	1.54	0.73
1:B:508:LEU:C	1:B:508:LEU:HD12	2.17	0.70
1:B:445:LEU:HG	4:B:711:IOD:I	2.63	0.69
1:B:532:ALA:O	1:B:536:GLU:HG3	1.92	0.69
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.41	0.68
1:A:236:MET:HE2	1:A:242:ALA:HB2	1.76	0.66
1:A:44:ALA:HB1	1:A:48:ASN:HB3	1.79	0.64
1:A:473:ILE:HD13	1:A:473:ILE:O	1.97	0.64
1:B:220:GLU:OE1	1:B:558:SER:OG	2.12	0.64
1:A:468:TYR:HB2	4:A:703:IOD:I	2.68	0.64
1:A:125:MET:HE1	1:A:133:LEU:HG	1.79	0.63
1:A:416:LEU:O	1:A:420:GLN:HG3	2.00	0.61
1:A:36:PRO:O	1:A:39:GLN:HG2	2.00	0.61
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.37	0.60
1:A:393:LEU:O	1:A:397:LEU:HB3	2.02	0.59
1:A:512:ASN:C	1:A:512:ASN:HD22	2.10	0.59
1:B:469:GLU:HB2	4:B:712:IOD:I	2.73	0.59
1:B:246:ASN:HD22	1:B:246:ASN:N	2.01	0.59
1:A:444:THR:O	1:A:445:LEU:HB2	2.03	0.58
1:A:66:GLN:O	1:A:69:SER:N	2.36	0.58
1:A:273:LEU:C	1:A:273:LEU:HD23	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:HD3	1:A:555:ALA:O	2.02	0.58
1:B:146:VAL:HG12	1:B:146:VAL:O	2.04	0.57
1:A:430:THR:HG22	1:A:431:ASN:N	2.20	0.57
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.86	0.57
1:B:601:VAL:HG21	4:B:704:IOD:I	2.75	0.57
1:A:491:THR:O	1:A:495:VAL:HG23	2.05	0.57
1:A:449:LEU:C	1:A:451:LYS:H	2.13	0.56
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.70	0.56
1:A:164:LYS:HA	1:A:164:LYS:HE3	1.88	0.56
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.52	0.56
1:A:431:ASN:H	1:A:431:ASN:HD22	1.54	0.56
1:A:444:THR:O	1:A:445:LEU:CB	2.54	0.55
1:A:245:LEU:HD13	1:A:269:LEU:HD21	1.88	0.55
1:B:246:ASN:HD22	1:B:246:ASN:H	1.54	0.54
1:A:245:LEU:HD13	1:A:269:LEU:CD2	2.36	0.54
1:A:46:ALA:HA	1:A:317:MET:HE2	1.88	0.54
1:A:419:VAL:O	1:A:423:VAL:HG23	2.08	0.54
1:B:315:THR:HG22	1:B:434:GLN:NE2	2.22	0.54
1:A:323:SER:O	1:A:328:GLY:N	2.41	0.53
1:A:66:GLN:C	1:A:69:SER:N	2.68	0.52
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.74	0.52
1:B:384:GLN:HG2	1:B:387:PHE:CE1	2.45	0.52
1:B:315:THR:HG22	1:B:434:GLN:HE21	1.74	0.52
1:A:207:GLY:O	1:A:246:ASN:HA	2.10	0.52
1:B:112:ARG:HD3	1:B:344:MET:HG2	1.91	0.52
1:A:146:VAL:CG1	1:A:146:VAL:O	2.58	0.51
1:A:35:ASN:C	1:A:35:ASN:HD22	2.19	0.51
1:A:512:ASN:ND2	1:A:515:LEU:H	2.08	0.51
1:A:121:PHE:HB3	1:A:134:TYR:CE2	2.45	0.51
1:A:451:LYS:N	1:A:451:LYS:HD3	2.26	0.51
1:B:273:LEU:C	1:B:273:LEU:HD23	2.35	0.51
1:B:6:ARG:HD3	1:B:555:ALA:O	2.11	0.51
1:B:146:VAL:HG13	1:B:343:ILE:CG2	2.40	0.51
1:A:456:ILE:HD12	1:A:458:SER:HB2	1.93	0.51
1:A:143:ARG:HH11	1:A:143:ARG:HB3	1.76	0.50
1:A:273:LEU:HD23	1:A:274:LEU:N	2.27	0.50
1:B:447:ILE:O	1:B:451:LYS:HB2	2.12	0.50
1:A:278:HIS:O	1:A:281:VAL:HG12	2.13	0.49
1:A:416:LEU:N	1:A:416:LEU:HD12	2.28	0.49
1:A:387:PHE:CD2	1:A:396:ILE:HD11	2.47	0.49
1:A:463:LEU:HD13	1:A:464:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLN:NE2	1:A:533:ARG:HH21	2.12	0.48
1:B:414:ASP:O	1:B:416:LEU:HD13	2.14	0.48
1:B:451:LYS:HA	1:B:451:LYS:CE	2.43	0.48
1:A:343:ILE:HA	1:A:362:GLY:HA3	1.96	0.48
1:A:431:ASN:H	1:A:431:ASN:ND2	2.11	0.48
1:A:246:ASN:N	1:A:246:ASN:HD22	2.11	0.48
1:A:272:THR:HA	1:A:295:ILE:HG21	1.96	0.48
1:B:127:GLY:O	4:B:712:IOD:I	3.02	0.47
1:A:46:ALA:HA	1:A:317:MET:CE	2.44	0.47
1:B:146:VAL:HG13	1:B:343:ILE:HG21	1.94	0.47
1:B:146:VAL:O	1:B:146:VAL:CG1	2.63	0.47
1:B:302:ALA:O	1:B:303:HIS:C	2.53	0.47
1:B:548:LEU:HD22	1:B:553:ARG:HG3	1.96	0.47
1:A:6:ARG:HD2	1:A:554:ALA:O	2.15	0.47
1:A:159:GLY:HA2	1:A:186:PHE:CE1	2.50	0.46
1:B:104:LEU:HD23	1:B:176:ILE:HB	1.96	0.46
1:B:444:THR:O	1:B:445:LEU:CB	2.63	0.46
1:A:271:GLU:O	1:A:272:THR:C	2.58	0.46
1:A:317:MET:SD	1:A:492:GLY:HA3	2.56	0.46
1:A:449:LEU:HD13	1:A:449:LEU:O	2.15	0.46
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.97	0.45
1:B:272:THR:HA	1:B:295:ILE:HG21	1.98	0.45
1:B:401:THR:HG22	1:B:403:ILE:H	1.80	0.45
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.62	0.45
1:A:228:GLN:HE22	1:B:228:GLN:NE2	2.12	0.45
1:B:445:LEU:CD1	1:B:450:LYS:HB3	2.37	0.45
1:B:167:ALA:O	1:B:168:ALA:C	2.60	0.45
1:B:508:LEU:C	1:B:508:LEU:CD1	2.89	0.45
1:A:414:ASP:O	1:A:415:ASN:CB	2.65	0.45
1:B:191:MET:HE2	1:B:191:MET:HA	1.99	0.45
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.52	0.44
1:B:225:THR:H	1:B:228:GLN:NE2	2.11	0.44
1:A:316:LEU:HD21	1:A:407:VAL:CG2	2.47	0.44
1:A:509:ARG:NH2	1:A:568:GLU:OE2	2.50	0.44
1:B:46:ALA:O	1:B:50:VAL:HG23	2.17	0.44
1:A:66:GLN:HA	1:A:66:GLN:OE1	2.18	0.44
1:A:416:LEU:O	1:A:420:GLN:CG	2.65	0.44
1:A:37:LEU:HD22	1:A:55:GLN:HE21	1.82	0.43
1:A:576:LEU:O	1:A:577:SER:C	2.61	0.43
1:A:396:ILE:O	1:A:399:SER:OG	2.34	0.43
1:A:37:LEU:HD22	1:A:55:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:O	1:A:143:ARG:C	2.61	0.43
1:A:530:SER:OG	1:A:533:ARG:HG3	2.19	0.43
1:B:6:ARG:H	1:B:6:ARG:HG2	1.64	0.43
1:B:529:GLN:NE2	1:B:533:ARG:HH21	2.15	0.43
1:A:45:ASP:OD1	1:A:45:ASP:C	2.61	0.43
1:A:214:ALA:O	1:A:227:ARG:HD3	2.19	0.42
1:B:193:CYS:HA	4:B:713:IOD:I	2.88	0.42
1:B:312:LYS:NZ	1:B:456:ILE:O	2.45	0.42
1:A:337:THR:HA	1:A:340:ILE:HD12	2.01	0.42
1:A:519:ALA:HB2	1:A:571:ILE:HD11	2.00	0.42
1:A:529:GLN:NE2	1:A:533:ARG:NH2	2.67	0.42
1:B:113:MET:HE2	1:B:113:MET:HA	2.01	0.42
1:B:447:ILE:HG13	1:B:448:PRO:HD3	2.01	0.42
1:A:30:ILE:HD12	1:A:210:PRO:HD3	2.02	0.42
1:A:317:MET:CE	1:A:496:LEU:HD11	2.50	0.42
1:A:390:GLU:O	1:A:393:LEU:N	2.53	0.42
1:A:146:VAL:O	1:A:146:VAL:HG12	2.19	0.42
1:A:267:LYS:O	1:A:268:ILE:C	2.63	0.42
1:A:456:ILE:HD12	1:A:458:SER:CB	2.49	0.42
1:A:569:GLN:O	1:A:570:VAL:C	2.61	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.91	0.41
1:A:246:ASN:HD22	1:A:246:ASN:H	1.66	0.41
1:A:474:GLN:O	1:A:478:ARG:HD3	2.20	0.41
1:A:53:LEU:HD12	1:A:488:THR:HG23	2.03	0.41
1:A:220:GLU:OE1	1:A:558:SER:OG	2.31	0.41
1:A:455:SER:O	1:A:456:ILE:O	2.38	0.41
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.21	0.41
1:B:523:LEU:HD23	1:B:523:LEU:HA	1.80	0.41
1:A:338:LEU:HD23	1:A:482:THR:OG1	2.20	0.41
1:A:433:ILE:HD12	1:A:453:PHE:CE1	2.55	0.41
1:B:15:GLU:HG3	1:B:18:LYS:HG3	2.02	0.41
1:B:414:ASP:O	1:B:416:LEU:N	2.54	0.41
1:A:36:PRO:O	1:A:39:GLN:CG	2.67	0.41
1:A:124:LEU:HA	1:A:472:PHE:CE2	2.55	0.40
1:A:461:TRP:HA	1:A:462:PRO:HD2	1.99	0.40
1:B:503:ASN:HD22	1:B:503:ASN:H	1.70	0.40
1:A:104:LEU:HD23	1:A:176:ILE:HB	2.03	0.40
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.36	0.40
1:B:410:PHE:O	1:B:437:ALA:HA	2.21	0.40
1:B:483:LYS:NZ	1:B:487:ASN:OD1	2.48	0.40
1:A:463:LEU:HD13	1:A:464:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/636 (91%)	532 (92%)	37 (6%)	10 (2%)	7	5
1	B	584/636 (92%)	554 (95%)	24 (4%)	6 (1%)	12	11
All	All	1163/1272 (91%)	1086 (93%)	61 (5%)	16 (1%)	9	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	A	445	LEU
1	A	456	ILE
1	B	415	ASN
1	A	454	PRO
1	A	462	PRO
1	B	127	GLY
1	B	445	LEU
1	A	199	ALA
1	B	446	PRO
1	B	449	LEU
1	A	336	GLN
1	A	434	GLN
1	B	168	ALA
1	A	446	PRO
1	A	447	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/542 (92%)	449 (90%)	49 (10%)	7	8
1	B	501/542 (92%)	465 (93%)	36 (7%)	13	15
All	All	999/1084 (92%)	914 (92%)	85 (8%)	10	11

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	ARG
1	A	21	LEU
1	A	25	GLU
1	A	35	ASN
1	A	39	GLN
1	A	66	GLN
1	A	95	LYS
1	A	98	ASP
1	A	143	ARG
1	A	146	VAL
1	A	172	ARG
1	A	185	PRO
1	A	198	THR
1	A	227	ARG
1	A	239	LYS
1	A	246	ASN
1	A	273	LEU
1	A	279	LYS
1	A	281	VAL
1	A	285	ILE
1	A	289	GLN
1	A	316	LEU
1	A	327	LYS
1	A	347	VAL
1	A	358	ARG
1	A	361	ARG
1	A	388	SER
1	A	394	THR
1	A	397	LEU
1	A	420	GLN
1	A	427	LYS
1	A	431	ASN

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Mol	Chain	Res	Type
1	A	434	GLN
1	A	440	THR
1	A	444	THR
1	A	445	LEU
1	A	451	LYS
1	A	463	LEU
1	A	464	LEU
1	A	465	PHE
1	A	473	ILE
1	A	478	ARG
1	A	499	LYS
1	A	503	ASN
1	A	512	ASN
1	A	533	ARG
1	A	557	ILE
1	A	605	LEU
1	B	1	MET
1	B	6	ARG
1	B	8	GLN
1	B	15	GLU
1	B	39	GLN
1	B	47	GLU
1	B	69	SER
1	B	72	GLN
1	B	95	LYS
1	B	126	LYS
1	B	130	GLN
1	B	131	LYS
1	B	143	ARG
1	B	166	VAL
1	B	239	LYS
1	B	241	LYS
1	B	246	ASN
1	B	273	LEU
1	B	304	GLN
1	B	327	LYS
1	B	337	THR
1	B	347	VAL
1	B	386	THR
1	B	402	GLU
1	B	416	LEU
1	B	434	GLN

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Mol	Chain	Res	Type
1	B	445	LEU
1	B	447	ILE
1	B	450	LYS
1	B	451	LYS
1	B	455	SER
1	B	457	ILE
1	B	467	GLU
1	B	469	GLU
1	B	503	ASN
1	B	548	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	55	GLN
1	A	91	GLN
1	A	190	GLN
1	A	196	ASN
1	A	246	ASN
1	A	309	GLN
1	A	336	GLN
1	A	431	ASN
1	A	474	GLN
1	A	477	GLN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	8	GLN
1	B	39	GLN
1	B	48	ASN
1	B	62	GLN
1	B	196	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	304	GLN
1	B	309	GLN
1	B	384	GLN
1	B	425	GLN
1	B	431	ASN
1	B	434	GLN

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Mol	Chain	Res	Type
1	B	503	ASN
1	B	529	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 25 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	S6P	B	702	-	15,15,15	1.45	2 (13%)	20,21,21	1.55	4 (20%)
2	MG0	B	701	-	34,34,34	2.04	5 (14%)	54,54,54	1.71	11 (20%)
6	SO4	B	717	-	4,4,4	0.71	0	6,6,6	0.55	0
5	GOL	A	714	-	5,5,5	0.91	0	5,5,5	0.99	0
3	S6P	A	702	-	15,15,15	1.28	4 (26%)	20,21,21	1.58	3 (15%)
2	MG0	A	701	-	34,34,34	1.72	3 (8%)	54,54,54	1.78	14 (25%)
6	SO4	B	718	-	4,4,4	0.77	0	6,6,6	0.48	0
6	SO4	B	719	-	4,4,4	0.54	0	6,6,6	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	S6P	B	702	-	-	1/20/20/20	-
2	MG0	B	701	-	-	0/40/50/50	0/3/3/3
5	GOL	A	714	-	-	3/4/4/4	-
3	S6P	A	702	-	-	1/20/20/20	-
2	MG0	A	701	-	-	1/40/50/50	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	MG0	O2-S1	7.03	1.51	1.43
2	B	701	MG0	C11-N2	-6.59	1.41	1.47
2	A	701	MG0	O2-S1	6.56	1.50	1.43
2	A	701	MG0	C11-N2	-4.45	1.43	1.47
2	B	701	MG0	C12-N2	-4.00	1.43	1.47
3	B	702	S6P	C2-C3	-3.46	1.47	1.53
2	A	701	MG0	O3-S1	3.01	1.46	1.43
3	A	702	S6P	C6-C5	2.56	1.55	1.51
3	A	702	S6P	P-O3P	2.31	1.57	1.50
3	B	702	S6P	C6-C5	2.26	1.54	1.51
3	A	702	S6P	C2-C3	-2.24	1.49	1.53
3	A	702	S6P	P-O1P	-2.20	1.46	1.54
2	B	701	MG0	C16-N4	-2.03	1.29	1.35
2	B	701	MG0	C8-C7	-2.02	1.51	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	MG0	C13-C12-N2	6.29	115.64	108.97
2	A	701	MG0	C12-N2-S1	-5.48	106.87	117.06
2	B	701	MG0	C12-N2-S1	-4.03	109.57	117.06
2	A	701	MG0	C13-C12-N2	3.75	112.94	108.97
2	A	701	MG0	C13-N1-C10	3.74	119.97	111.57
2	B	701	MG0	O3-S1-N2	-3.68	103.22	106.69
3	B	702	S6P	O6-P-O3P	3.68	116.38	106.44
3	A	702	S6P	O2P-P-O6	3.56	115.96	106.67
2	B	701	MG0	C12-N2-C11	-3.44	108.17	112.12
2	B	701	MG0	C11-N2-S1	-3.43	110.69	117.06
2	A	701	MG0	C12-N2-C11	-3.28	108.35	112.12
2	A	701	MG0	C11-N2-S1	-3.16	111.18	117.06
2	B	701	MG0	C14-S1-N2	3.09	111.01	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	MG0	O3-S1-O2	-2.87	115.11	119.59
2	A	701	MG0	O2-S1-N2	2.69	109.22	106.69
2	A	701	MG0	C14-C15-N3	-2.65	119.96	123.19
2	A	701	MG0	F4-C8-C7	-2.53	107.09	111.84
2	B	701	MG0	F5-C8-C7	-2.49	107.15	111.84
2	A	701	MG0	F1-C9-F3	2.42	114.89	107.54
3	B	702	S6P	C6-C5-C4	-2.41	107.67	112.22
2	B	701	MG0	C18-C14-S1	2.41	122.13	119.73
2	A	701	MG0	F3-C9-C7	-2.38	107.36	111.84
3	A	702	S6P	C1-C2-C3	-2.36	107.36	112.17
3	A	702	S6P	O6-P-O3P	-2.34	100.12	106.44
2	B	701	MG0	F5-C8-F4	2.33	114.61	107.54
3	B	702	S6P	O3-C3-C2	2.26	114.07	108.93
2	A	701	MG0	O3-S1-N2	-2.15	104.66	106.69
2	A	701	MG0	C3-C4-C5	2.12	122.99	120.30
3	B	702	S6P	C1-C2-C3	-2.07	107.95	112.17
2	B	701	MG0	C12-C13-N1	2.06	115.12	110.78
2	B	701	MG0	F3-C9-C7	-2.06	107.97	111.84
2	A	701	MG0	O1-C7-C9	2.02	110.74	106.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

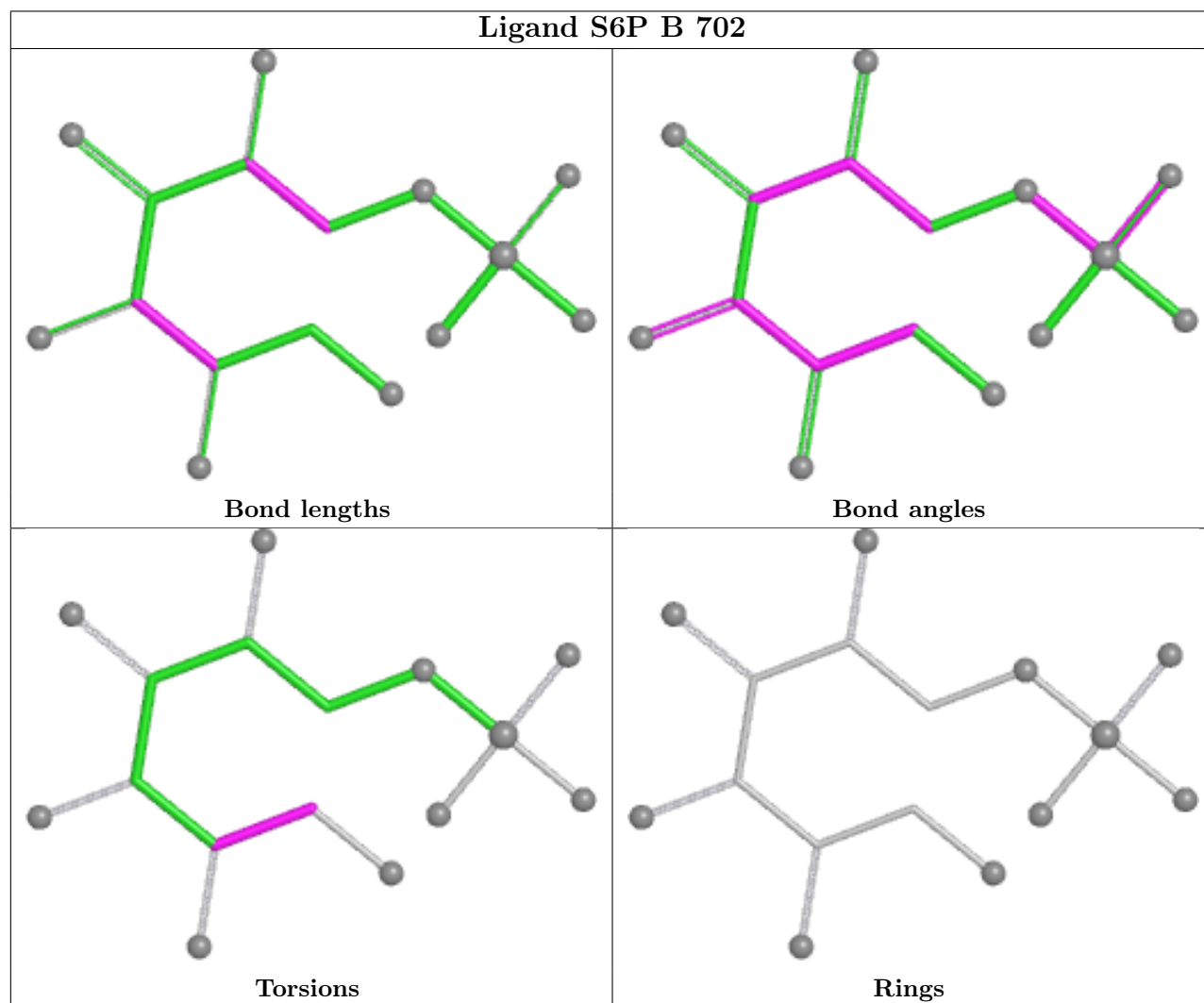
Mol	Chain	Res	Type	Atoms
5	A	714	GOL	C1-C2-C3-O3
5	A	714	GOL	O1-C1-C2-C3
5	A	714	GOL	O2-C2-C3-O3
2	A	701	MG0	C12-N2-S1-O3
3	B	702	S6P	O1-C1-C2-O2
3	A	702	S6P	C6-O6-P-O3P

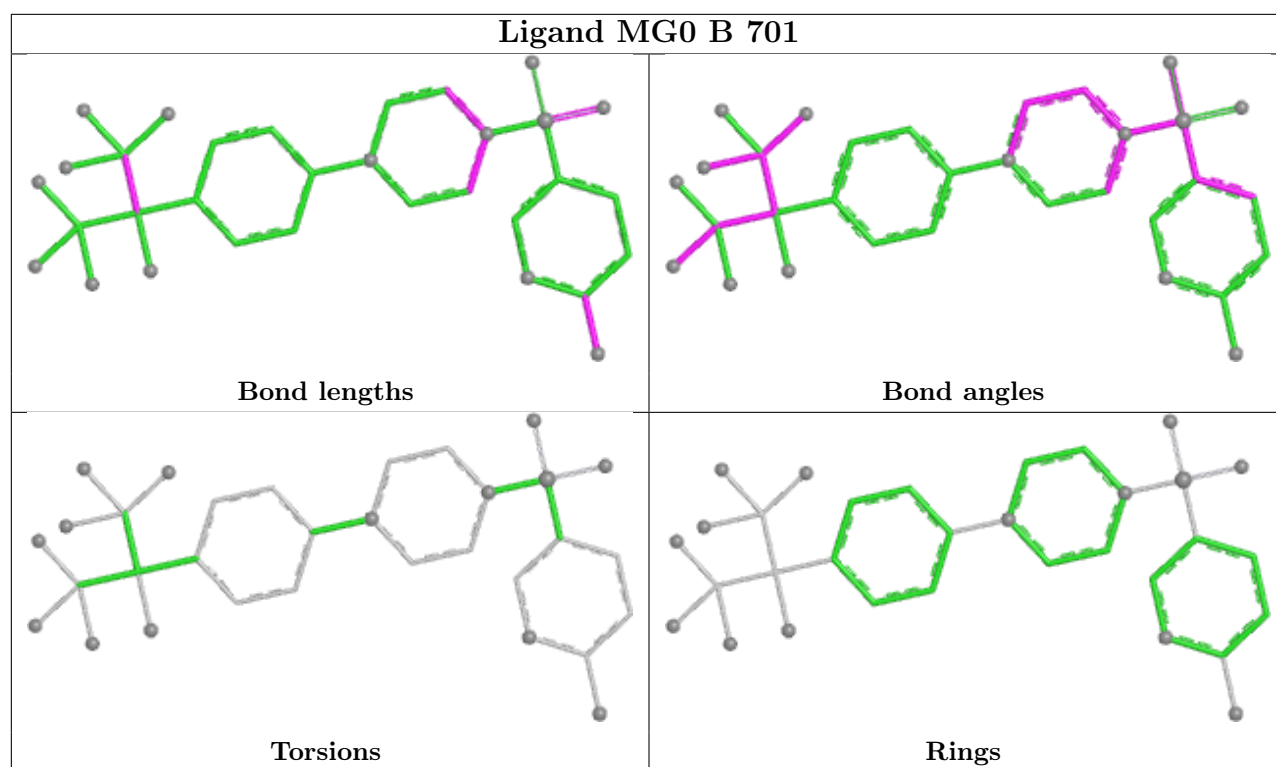
There are no ring outliers.

No monomer is involved in short contacts.

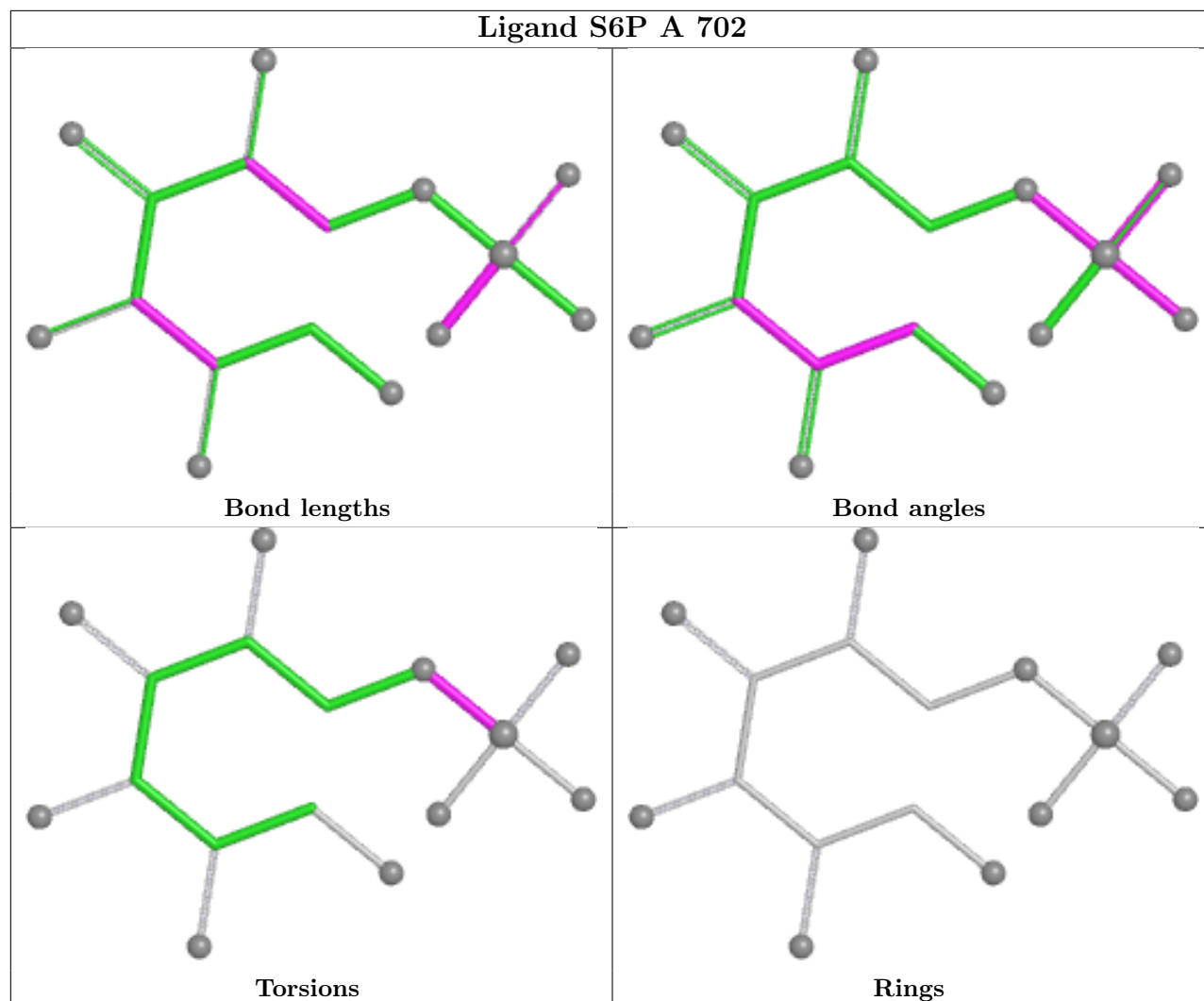
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

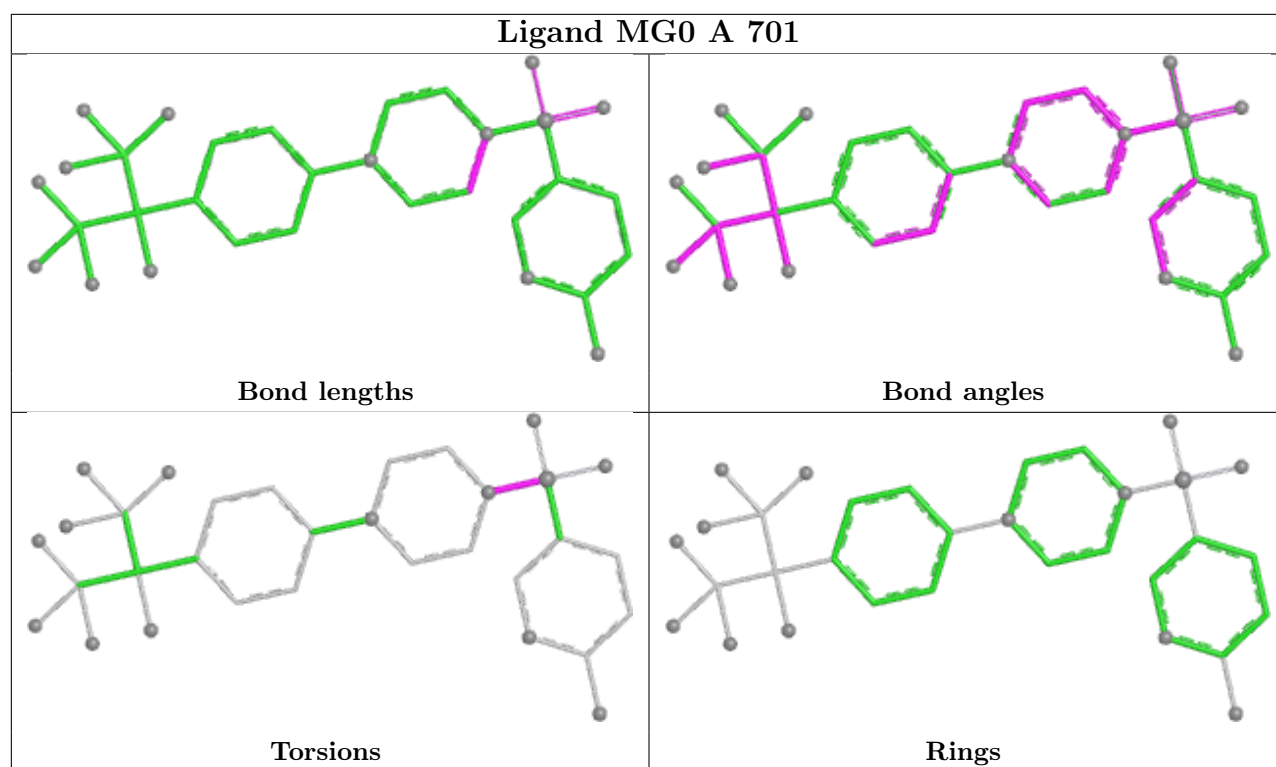
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand S6P A 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/636 (91%)	0.51	38 (6%) 25 22	30, 50, 82, 118	0
1	B	590/636 (92%)	0.17	16 (2%) 56 53	27, 45, 71, 111	0
All	All	1175/1272 (92%)	0.34	54 (4%) 37 34	27, 47, 79, 118	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LEU	6.7
1	A	387	PHE	5.2
1	B	447	ILE	5.0
1	A	465	PHE	4.3
1	B	21	LEU	3.8
1	A	448	PRO	3.8
1	A	430	THR	3.6
1	B	448	PRO	3.4
1	A	452	LEU	3.3
1	A	447	ILE	3.3
1	A	357	PHE	3.2
1	B	465	PHE	3.1
1	B	381	GLN	3.1
1	A	464	LEU	3.1
1	A	403	ILE	3.0
1	A	358	ARG	3.0
1	A	393	LEU	3.0
1	A	397	LEU	2.9
1	A	386	THR	2.9
1	A	65	GLY	2.9
1	A	429	LYS	2.9
1	B	445	LEU	2.8
1	A	463	LEU	2.8
1	A	454	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	466	PHE	2.7
1	A	467	GLU	2.6
1	B	454	PRO	2.6
1	A	69	SER	2.5
1	A	235	LYS	2.5
1	B	66	GLN	2.5
1	B	449	LEU	2.4
1	B	70	THR	2.4
1	B	357	PHE	2.4
1	A	441	VAL	2.4
1	B	441	VAL	2.4
1	A	412	LEU	2.4
1	A	282	ASP	2.3
1	A	400	LEU	2.3
1	A	365	ILE	2.3
1	A	469	GLU	2.3
1	A	450	LYS	2.2
1	A	445	LEU	2.2
1	A	385	PHE	2.2
1	B	450	LYS	2.2
1	A	21	LEU	2.1
1	B	168	ALA	2.1
1	B	1	MET	2.1
1	A	5	LYS	2.1
1	A	408	PHE	2.1
1	A	131	LYS	2.1
1	A	66	GLN	2.1
1	A	420	GLN	2.1
1	B	460	THR	2.0
1	A	410	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

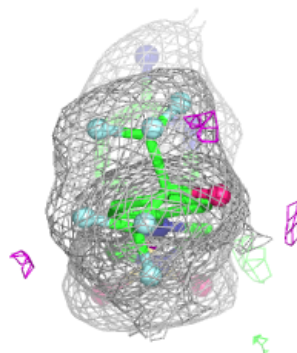
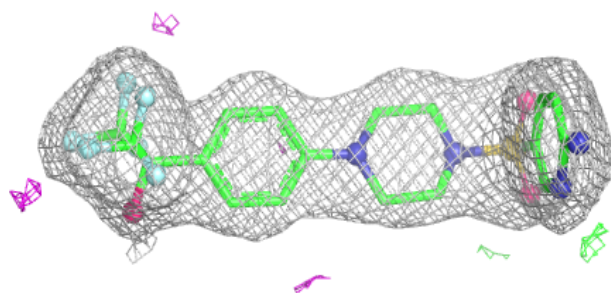
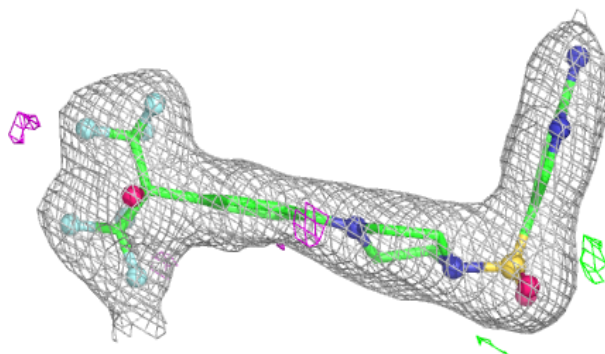
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	B	717	5/5	0.75	0.11	70,72,78,92	0
5	GOL	A	714	6/6	0.77	0.16	45,48,51,57	0
6	SO4	B	719	5/5	0.77	0.13	76,78,88,93	0
4	IOD	A	713	1/1	0.84	0.13	61,61,61,61	1
6	SO4	B	718	5/5	0.86	0.09	66,68,71,94	0
4	IOD	A	712	1/1	0.90	0.12	88,88,88,88	1
4	IOD	B	711	1/1	0.90	0.10	81,81,81,81	1
4	IOD	B	712	1/1	0.92	0.08	75,75,75,75	1
4	IOD	B	714	1/1	0.92	0.14	65,65,65,65	1
4	IOD	A	706	1/1	0.93	0.11	86,86,86,86	0
4	IOD	A	709	1/1	0.93	0.11	83,83,83,83	1
4	IOD	A	711	1/1	0.93	0.10	67,67,67,67	1
4	IOD	A	703	1/1	0.93	0.09	74,74,74,74	0
4	IOD	B	710	1/1	0.94	0.11	89,89,89,89	1
4	IOD	B	716	1/1	0.94	0.07	66,66,66,66	1
4	IOD	B	713	1/1	0.94	0.09	64,64,64,64	1
4	IOD	B	708	1/1	0.95	0.11	66,66,66,66	1
4	IOD	B	709	1/1	0.95	0.13	90,90,90,90	0
4	IOD	A	707	1/1	0.95	0.09	65,65,65,65	1
4	IOD	A	708	1/1	0.95	0.13	81,81,81,81	1
4	IOD	A	710	1/1	0.96	0.05	61,61,61,61	1
4	IOD	B	703	1/1	0.96	0.06	55,55,55,55	0
4	IOD	B	707	1/1	0.97	0.07	64,64,64,64	0
2	MG0	B	701	32/32	0.97	0.06	29,34,41,42	0
3	S6P	B	702	16/16	0.97	0.05	24,29,32,33	0
4	IOD	B	706	1/1	0.97	0.06	56,56,56,56	0
4	IOD	B	715	1/1	0.97	0.05	69,69,69,69	1
2	MG0	A	701	32/32	0.98	0.06	32,37,42,43	0
3	S6P	A	702	16/16	0.98	0.05	28,33,38,41	0
4	IOD	A	704	1/1	0.98	0.06	60,60,60,60	0
4	IOD	A	705	1/1	0.98	0.07	51,51,51,51	1
4	IOD	B	705	1/1	0.99	0.06	51,51,51,51	1
4	IOD	B	704	1/1	0.99	0.04	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

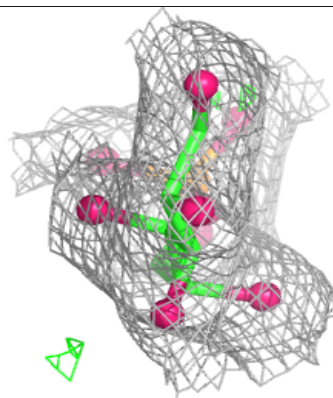
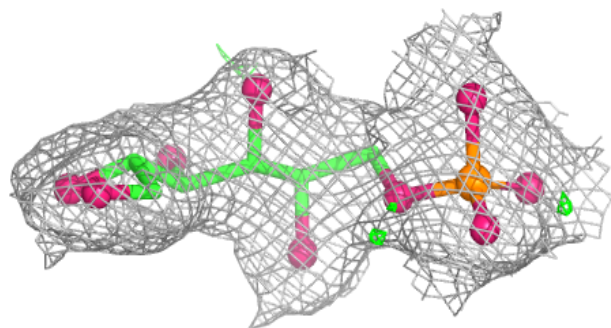
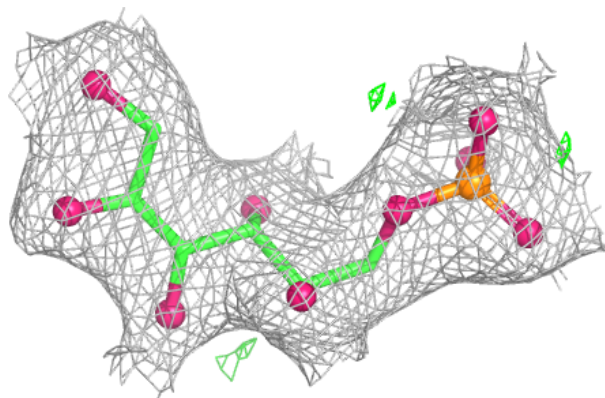
Electron density around MG0 B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



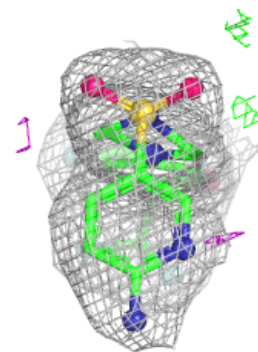
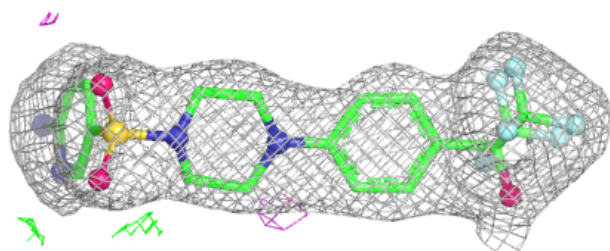
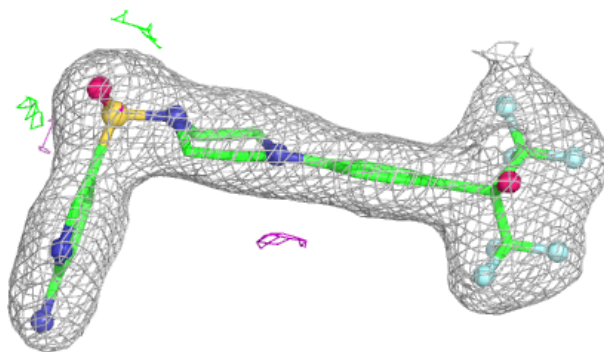
Electron density around S6P B 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

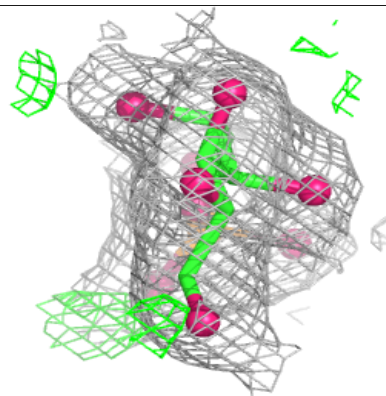
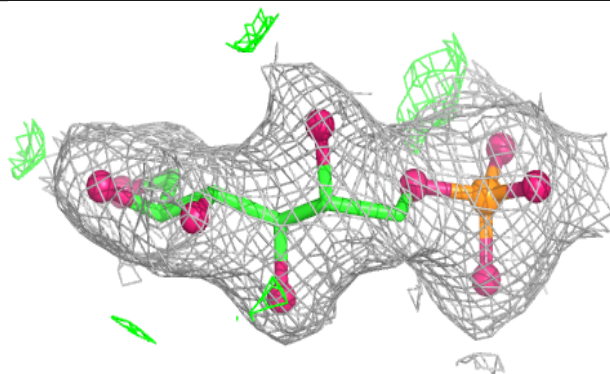
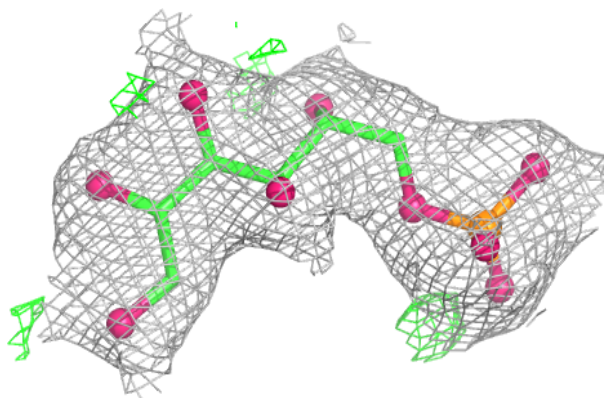


Electron density around MG0 A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around S6P A 702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.